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Compiling, linking and running a “test case” code on a parallel Linux environment for HPC

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Information & Communication Technology Section (ICTS)

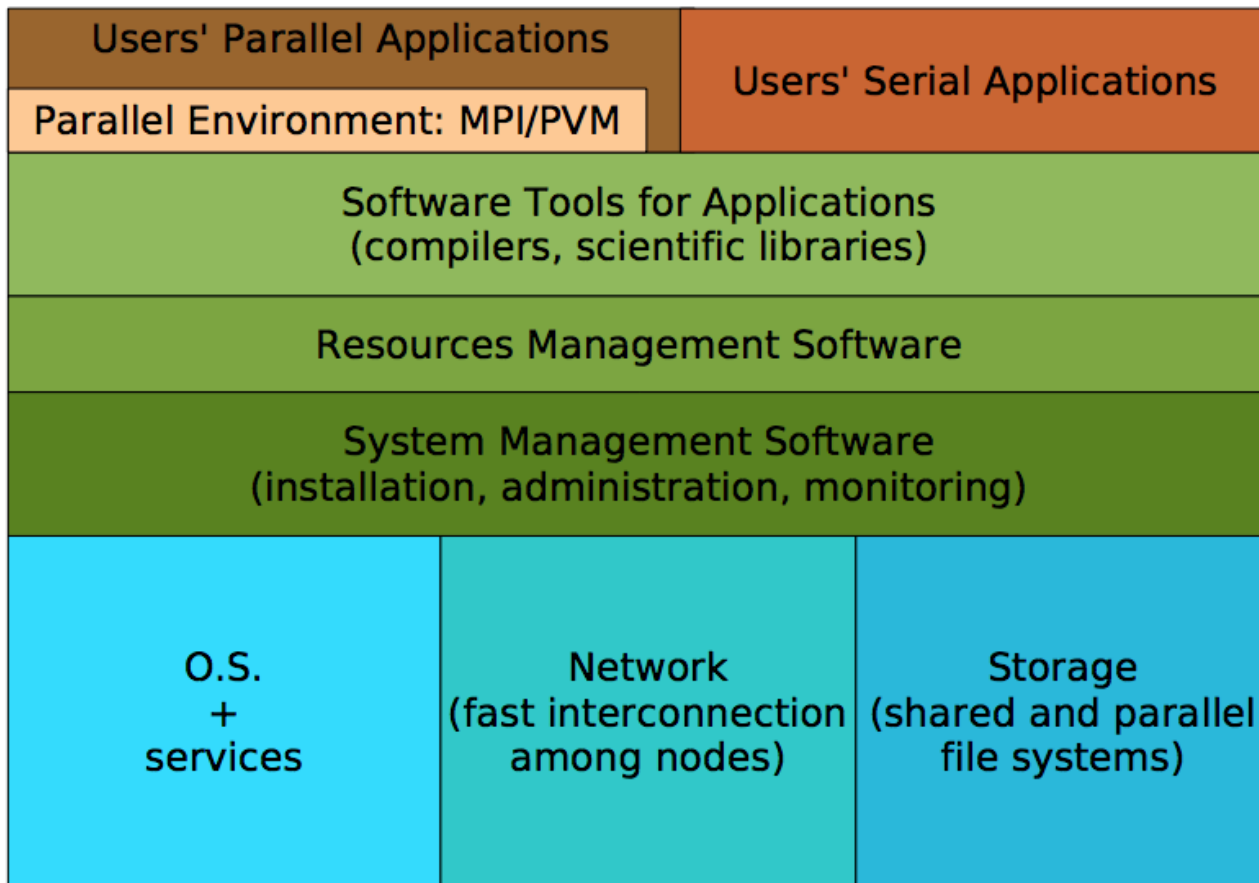
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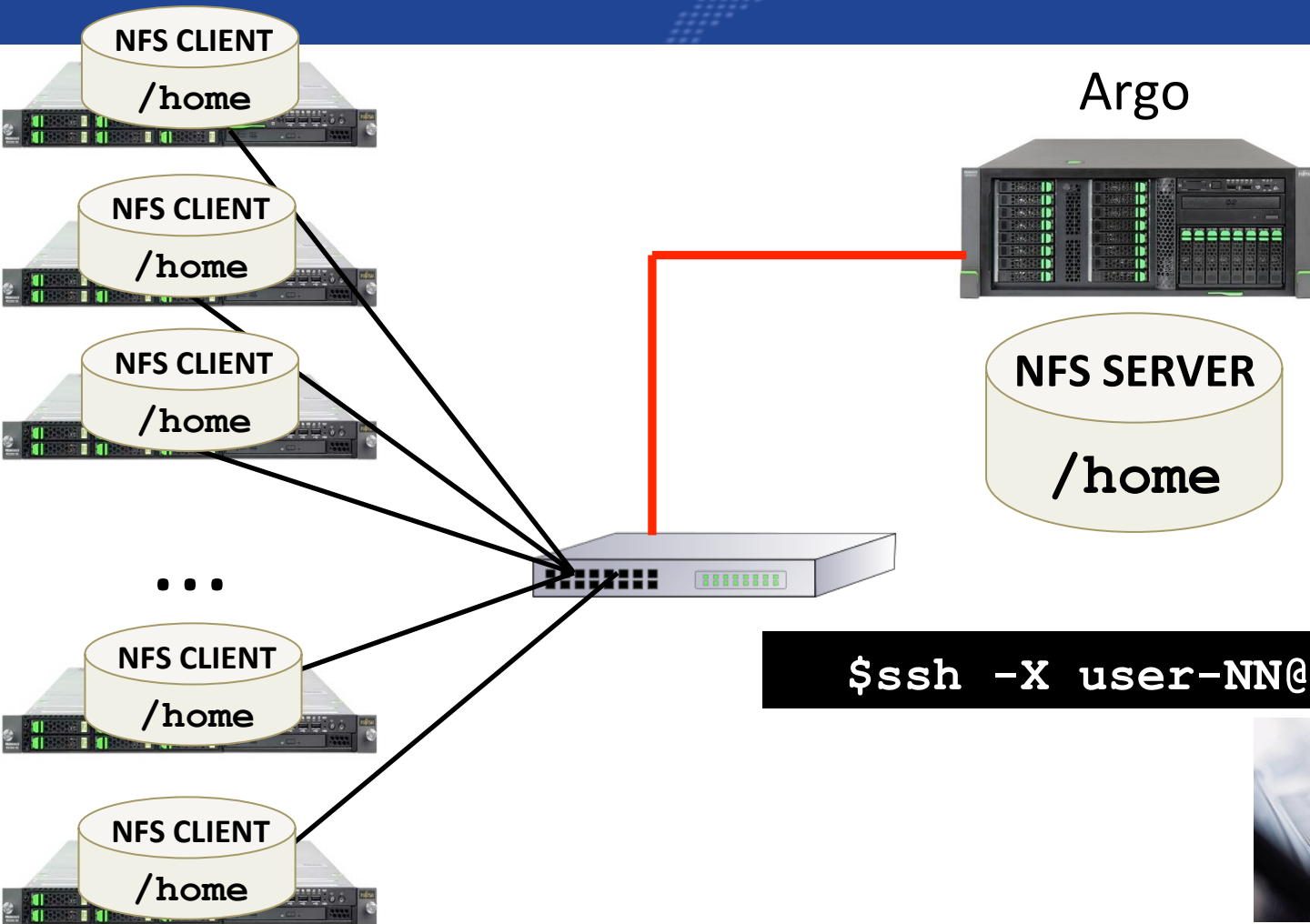


Outline

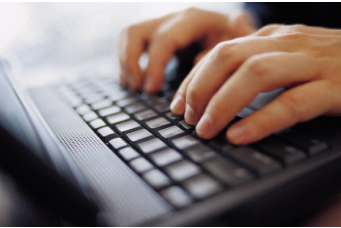
- The Argo Parallel System
- The Batch System
- Shell Script for Submission
- Serial Execution
- Parallel Execution

HPC Infrastructure Layers





```
$ssh -X user-NN@argo.ictp.it
```



N = 01, 02, ..., 30



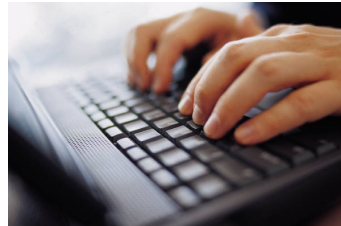
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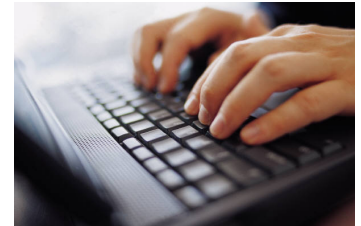
...



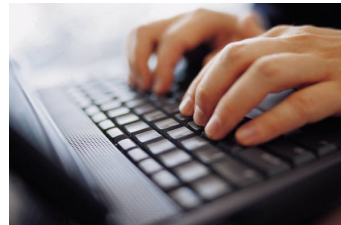
[user-1@argo ~]\$



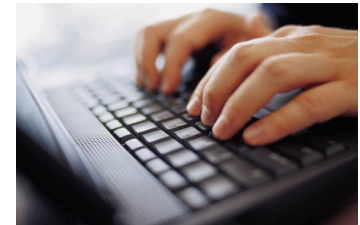
[user-2@argo ~]\$



[user-3@argo ~]\$



[user-5@argo ~]\$





The Resource Manager

- Service based on a server (master) and many clients (compute nodes) model
- Handles fair sharing among a number of users that aim to run a number of jobs
- Filter the access to the compute nodes
- Schedules the next job to be executed
- Enhances the configuration of the system policies
- Maui and Torque are the two tools used for resource management on Argo



1) Create the submission script

3 fundamental steps
for job execution

```
[user-1@argo ~]$ more sub_script.sh
```

```
#!/bin/bash
#PBS -l nodes=1:ppn=12
#PBS -l walltime=00:10:00
#PBS -q smr2626

cd $PBS_O_WORKDIR

./my_prog.x
```

2) Submit the script

```
[user-1@argo ~]$ qsub sub_script.sh
70.argo
```

3) Monitor job execution

```
[user-1@argo ~]$ qstat -u $USER
```

Job id	Name	User	Time Use	S	Queue
70.argo	test_pbs	user-1	0	R	smr2626



1) Create the submission script

3 fundamental steps
for job execution

```
[user-1@argo ~]$ more sub_script.sh
```

```
#!/bin/bash
#PBS -l nodes=1:ppn=12
#PBS -l walltime=00:30:00
#PBS -q smr2626

cd $PBS_O_WORKDIR

module load openmpi/...

mpirun ./my_prog.x
```

2) Submit the script

```
[user-1@argo ~]$ qsub sub_script.sh
70.argo
```



3) Monitor job execution

```
[user-1@argo ~]$ qstat -u $USER
```

Job id	Name	User	Time Use	S	Queue
70.argo	test_pbs	user-1	0	R	smr2626



Modulefiles Motivation

- On HPC cluster it is often desirable to have multiple version of the same software installed
- Changing environment variables like \$PATH manually to accommodate this is tedious
- Corresponding shell scripts would have to be written for multiple languages
- All of these explicit steps are error prone and difficult to maintain
- There is no simple upgrade path



Module Commands

- module avail
 - Display the current available module tree
- module list
 - Display currently loaded modules
- module purge
 - Deletes all modules from list of loaded



Module Commands

- module load <package>
 - Loads the current default module of package
- module unload
 - Remove module package from the environment
- module show <package>
 - Displays command triggered by module load
- module help package



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Have fun!!

